

Phase diagram of dipolar bosons in 2D with tilted polarization

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We analyze the ground state of a system of dipolar bosons moving in the XY plane and such that their dipolar moments are all aligned in a fixed direction in space. We focus on the general case where the polarization field forms a generic angle α with respect to the Z axis. We use the Path Integral Ground State method to analyze the static properties of the system as both α and the density n vary over a wide range where the system is stable. We use the maximum of the static structure function as an order parameter to characterize the different phases and the transition lines among them. We find that aside of a superfluid gas and a solid phase, the system reaches a stripe phase at large tilting angles that is entirely induced by the anisotropic character of the interaction. We also show that the quantum phase transition from the gas to the stripe phase is of second order, and report approximate values for the critical exponents.

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In recent years, dipolar Bose gases have received much attention. The study of quantum degenerate gases of dipolar species has become one of the most active areas of experimental and theoretical research in the field of ultracold atoms [1–3]. From the theoretical point of view, the anisotropic and long range character of the interaction make dipolar systems unique, exhibiting features like p -wave superfluidity in two-dimensional (2D) Fermi gases [4] or roton instability [5–7]. These two properties of the dipole-dipole potential enrich the phase diagram when compared with other systems with more common isotropic interactions of the Van der Waals type. In this way, the realization of systems featuring strong dipolar forces opens prospects for investigating new and highly interesting many-body effects, not present in other systems.

Up to now, most of the theoretical work on dipolar systems in two dimensions have focused on the most simple case where the dipolar moments are all aligned in the normal direction to the plane where they move. Less attention has been paid to the more general situation where dipoles are polarized along an arbitrary direction, including the analysis of scattering properties [8] or the superfluid and collapse instabilities of a quasi-two-dimensional gas of dipolar fermions aligned by an external field [9]. One remarkable feature induced by the anisotropy of the interaction is the emergence of a stripe phase, which has been predicted to appear both in Bose [7] and Fermi [11–13]. Some of these calculations were done in the mean field approximation, predicting the appearance of stripes even in the isotropic case where all dipoles are polarized perpendicularly to the plane of movement, although recent Monte Carlo calculations arrived to different conclusion [10]. In this letter we address this topic and characterize the existence of the stripe phase as a function of the density and polarization angle for the Bose case, and determine the corresponding solid and gas transition lines.

In previous works we discussed the low-density properties [14] and elementary excitation spectrum [7] of the fully anisotropic 2D dipolar interaction. In this Letter we extend the analysis and investigate the phase diagram of a 2D system of bosonic dipoles tilted by an angle α with respect to the normal direction to the plane where they move. The tilting angle is assumed to be produced by an external polarization field that makes all the dipoles tightly point along a fixed direction in space. We omit any kind of second order interactions between the dipoles and the polarization field, so the net effect of the latter is to simply orient them along a fixed direction in space.

In contrast to the particular $\alpha = 0$ case, the dipole-dipole interaction is in general fully anisotropic. This property brings additional degrees of freedom which make possible a stable stripe phase. Using first-principles quantum Monte Carlo we have established in this work the phase diagram of bosonic tilted dipoles in 2D and characterized the phase transitions between the gas, crystal and stripe phases.

The model Hamiltonian describing a system of N polarized and interacting dipoles is written as

$$H = -\frac{\hbar^2}{2m} \sum_{j=1}^N \nabla_j^2 + \frac{C_{dd}}{4\pi} \sum_{i<j}^N \left[\frac{1 - 3\lambda^2 \cos^2 \theta_{ij}}{r_{ij}^3} \right], \quad (1)$$

where C_{dd} is proportional to the square of the (magnetic μ or electric d) dipole moment, and $\lambda = \sin \alpha$. Polar coordinates (r_{ij}, θ_{ij}) describe the separation between particles i th and j th, respectively. In the following we use dimensionless units obtained from the characteristic dipolar length $r_0 = mC_{dd}/(4\pi\hbar^2)$ and energy $\varepsilon_0 = \hbar^2/(mr_0^2)$.

We perform stochastic Path Integral Ground State (PIGS) [15] calculations in order to build the $T = 0$ phase diagram of the system as a function of the dipolar density nr_0^2 and polarization angle α . We simulate a finite number of particles N in a box of area $A = N/(nr_0^2)$ with periodic boundary conditions. One relevant feature, already present in the two-body problem, is the fact that,

in the absence of additional two-body forces, the system can only be stable when the dipolar interaction is strictly non-negative. In this way, there is a critical tilting angle $\alpha_c \simeq 0.61$ above which the system collapses because the interaction produces regions where it becomes attractive.

The efficiency of the PIGS method is largely enhanced when a suitable variational wave function is used at the end points of the chains representing the interacting particles. Anyway, it is important to remark that estimations of any observable in PIGS are unbiased with respect to that trial wave function and that, even without it, the results remain unchanged [16]. We have checked that, despite the fact that the interaction is anisotropic, the trial wave function does not need to explicitly incorporate that feature, and we have chosen a standard Jastrow product

$$\Psi_T(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \prod_{i < j} f(r_{ij}), \quad (2)$$

with the two-body correlation factor given by

$$f(r) = \begin{cases} K_0(2/\sqrt{r}) & \text{if } r \leq R_M \\ B \exp \left[- \left(\frac{C}{r} + \frac{C}{L-r} \right) \right] & \text{if } r > R_M \end{cases} \quad (3)$$

where B, C and R_M are constants to be fixed at each density and tilting angle, and L is the side of the simulation box. By imposing $f(L/2)$ to be 1, and $f(r)$ and $f'(r)$ to be continuous at $r = R_M$, only R_M remains unknown, and we determine its value through a variational optimization. The two-body correlation factor $f(r)$ built in this way reproduces the exact behavior of the zero-energy solution of the $\alpha = 0$ two-body problem at short distances, matched with the box-symmetrized form of a phononic wave function in two dimensions [17].

We know that for $\alpha = 0$ the system remains in gas phase up to a freezing density $nr_0^2 \sim 290$, where the system undergoes a first order phase transition to a triangular solid [18, 19]. A similar behavior happens when the polarization angle increases, although the transition density changes with α . In our simulation we still use Eqs. (2) and (3) at the end points of the PIGS chains in the crystal phase, but in this case the starting configuration correspond to the sites of the triangular lattice that optimally describe the system. This corresponds to an equilateral triangular lattice at $\alpha = 0$, but that changes when α increases, squeezing the fundamental triangle of the lattice in such a way that the distance between particles in the direction parallel to the projection of the dipolar moment on the plane is reduced. Our results for the deformation angles at each angle α are compatible with classical Monte Carlo simulations where the potential energy of the system is minimized.

In order to characterize the gas-solid transition we use the maximum strength of the static structure factor divided by the number of particles in the simulation as an order parameter, $\eta = S_{max}(\mathbf{k})/N$ [20]. Figure 1 shows

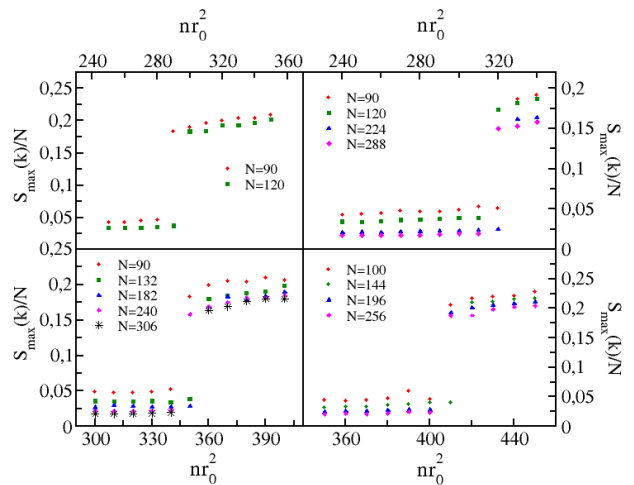


FIG. 1: (color online). Evolution of the order parameter $S_{max}(\mathbf{k})/N$ with the density for $\alpha = 0.1$ (upper left), $\alpha = 0.2$ (upper right), $\alpha = 0.3$ (lower left) and $\alpha = 0.4$ (lower right) for an increasing number of particles N .

η as a function of the density for the polarization angles $\alpha = 0.1, 0.2, 0.3, 0.4$ and different number of particles in the simulation. One can clearly see from the figure that up to a certain density the order parameter is zero, corresponding to a phase where the main peak in $S(\mathbf{k})$ does not increase significantly with the number of particles. At higher densities, though, η approaches a constant non-zero value, revealing the existence of a main Bragg peak. The discontinuity point indicates the transition density at which crystallization takes place. Table I shows the transition densities for several tilting angles α , while γ stands for the deformation angle, defined in terms of the primitive vectors of the Bravais lattice

$$\mathbf{a}_1 = a\hat{i}, \quad \mathbf{a}_2 = \frac{a}{2}(\hat{i} + \hat{j}\tan\gamma) \quad (4)$$

with a fixed by the density. One sees from the table that the transition density increases with the polarization angle, due to the fact that, overall, the strength of the interaction decreases when α increases. Being the gas-crystal transition of first order, there are two densities (freezing and melting) defining the coexistence region. In the current case these two densities must be quite close to each other as we have not been able to resolve them from our simulations, as happened also in the isotropic case [18]. Finally we have checked that the gas-crystal transition line is well characterized by a parabolic curve of the form $n_c r_0^2 = a + b \sin^2 \alpha$, with $a = 281.75 \pm 2.75$ and $b = 836.41 \pm 34.38$.

By increasing further the tilting angle a new ordered phase appears. This new phase, characterized by the arrangement of particles in stripes along the direction where the interaction presents weakest strength, has been reported to exist in Bose [7] and Fermi [11–13] systems of 2D dipoles. The stripe phase is characterized by the

α	0.0	0.1	0.2	0.3	0.4
γ	60°	60°	60°	62°	64°
$n_c r_0^2$	280(20)	290(20)	320(20)	350(20)	410(20)

TABLE I: Tilting angle α , deformation angle γ and transition densities $n_c r_0^2$ of the gas-crystal transition.

emergence of Bragg peaks in $S(\mathbf{k})$ due to the spatial ordering in one direction compared with the gas phase. For this reason we also use here the η parameter defined above in order to characterize now the transition from gas to stripes. The upper and lower left panels of Fig. 2 show the evolution of η with the density for $\alpha = 0.54$ and 0.58 , respectively, and for different number of particles in the simulation. The different behavior when compared with the gas-crystal transition is evident and shows that the transition is in this case continuous. As we are always simulating a finite system in a box with periodic boundary conditions, we use finite size scaling near the transition point in order to find the critical exponents of this second-order phase transition. We thus employ the following form of a length-scaled order parameter

$$\eta_L(t) = L^{-\beta/\nu} \tilde{\eta}(L^{1/\nu} t) \quad (5)$$

corresponding to a system of box side L . In this expression $t = (n - n_c)/n_c$ is the reduced density around the critical point, while ν and β stand for the critical exponents of the order parameter and the correlation length, respectively, the later scaling as $t^{-\nu}$ [21]. In our case we find ν and β as the optimal values that collapse all curves to a single $\tilde{\eta}$ line. We have found that the best agreement is achieved for $\nu = 0.33$ and $\beta = 0.63$. The upper and lower right panels in Fig. (2) show the collapse of the data in the respective left panels when these values are used. As it can be seen, the scaling of the data is nicely reproduced, although it is difficult to accurately determine the exact value of the critical exponents from the Monte Carlo data.

An interesting result provided by the finite size scaling analysis is the fact that the values of the critical exponents do not show a significant dependence on the polarization angle α . In this way, and for $\alpha \geq 0.45$, only the transition density changes when α varies. The values of ν and β derived from our results are compatible with the classical 3D Ising universality class, $\beta = 0.326$ and $\nu = 0.630$, associated to the $U(1)/Z_2$ symmetry breaking arising when the stripes disappear, bearing in mind that the critical behavior of a quantum system in d dimensions is equivalent to that of the corresponding classical system in $d + 1$ dimensions [22]. The finite size scaling analysis of the results for different tilting angles allows for the determination of the gas-stripe transition line, which we summarize in Table II. This line turns out to be well fitted by a curve of the form $n_c r_0^2 = n_0 r_0^2 + a \sin^2(\alpha - \alpha_0)$ with $n_0 r_0^2 = 125.59 \pm 3.70$, $a = 18750 \pm 2113$ and $\alpha_0 = 0.6047 \pm 0.0052$.

It is interesting to notice that the emergence of a stripe

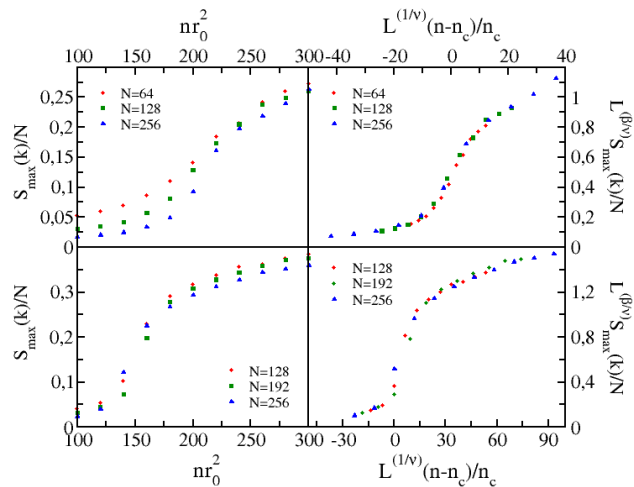


FIG. 2: (color online). Order parameter η for $\alpha = 0.54$ and 0.58 as a function of the dipolar density (upper and lower left panels, respectively).

α	0.52	0.54	0.56	0.58	0.60
$n_c r_0^2$	260(20)	205(20)	160(20)	140(20)	125(20)

TABLE II: Tilting angle α and transition densities $n_c r_0^2$ of the gas-stripe transition.

phase is entirely due to the anisotropy of the interaction, but that this ordering effect is in direct competition with other natural disordering sources like quantum fluctuations. As a consequence, the appearance of a stripe phase imposes severe conditions on the system, in particular on the existence of a threshold density and polarization angle. At lower densities than those shown in the table the system remains in gaseous phase for all values of α up to the collapse limit.

We end the analysis describing the high density and high polarization angle region. We have seen that for low and intermediate values of α the system remains in solid phase at high densities, while stripes appear when α is larger than some critical angle. Consequently, there is a crystal to stripe transition line at an intermediate region. Getting this transition well characterized is difficult from the simulation because the system changes from one high density ordered phase to another. Still, the different arrangement in each phase can be observed in the static structure factor $S(\mathbf{k})$: the solid phase is characterized by an infinite number of Bragg peaks located at the characteristic vectors of the reciprocal lattice, while this is not the case in the stripe phase where ordering appears in only one direction.

The upper panels in Fig. 3 show a typical example of the full $S(\mathbf{k})$ in the stripe and solid phases as obtained from our PIGS simulations. As it can be seen, a second peak is clearly resolved in the solid phase in comparison with the stripe phase, where a single Bragg peak asso-

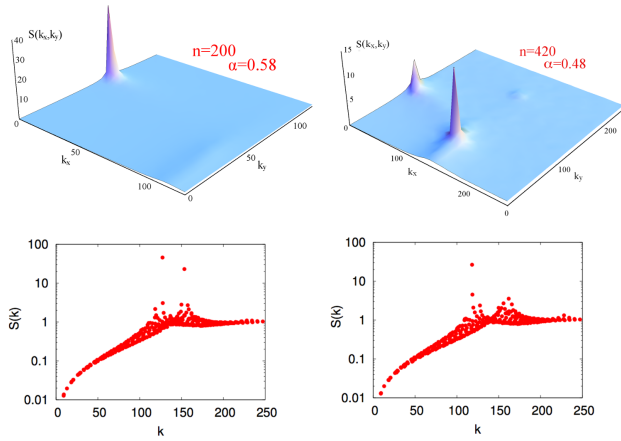


FIG. 3: (color online). Typical form of the static structure factor $S(\mathbf{k})$ of the system in the stripe and solid phases (left and right upper panels, respectively). The lower panels show the projected $S(\mathbf{k})$ for a density $nr_0^2 = 450$ and tilting angles $\alpha = 0.48$ (left) and $\alpha = 0.48125$ (right).

nr_0^2	450	480	500	550
α_c	0.4806(1)	0.4819(1)	0.4819(1)	0.4838(1)

TABLE III: Densities and tilting angles corresponding to the solid-stripe transition.

ciated to the periodicity along the Y axis is visible. In fact the figure already shows a third peak in the solid phase that has however much less strength but that, together with the other two, put in evidence the structure of the triangular lattice. All these peaks are expected to get more strength when the number of particles in the simulation increases.

In this way, we characterize the stripe to solid phase transition from the emergence of a second Bragg peak in the simulation, absent in the former but present in the latter. In order to describe the solid-stripe phase transition we have performed several PIGS simulations with slightly different values of α and nr_0^2 , and have determined through the analysis of the peak structure of $S(\mathbf{k})$ the polarization angle that makes the system lose crystalline order. The lower panels in Fig. 3 show the emergence of the second Bragg peak for a density $nr_0^2 = 450$ with $\alpha = 0.48$ (left) and $\alpha = 0.48125$ (right). The figure shows the *projected* $S(\mathbf{k})$ where the full 2D $S(\mathbf{k})$ is represented in a single plot with the magnitude of \mathbf{k} on the X axis. The emergence of the second Bragg peak is quite abrupt and allows finding the solid to stripe transition point at each fixed density. The results obtained with this method are shown in Table III. It is remarkable how steep the curve is, thus indicating that the stripe phase seems to be the stable one up to extremely large densities that are out of reach of our numerical simulations.

An obvious question that arises at this point regards

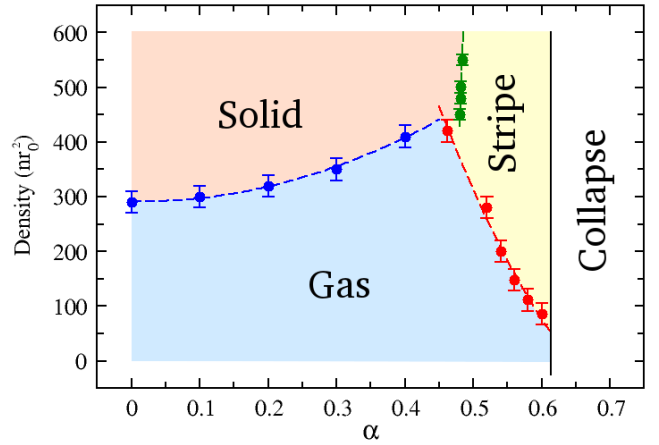


FIG. 4: (color online). Evolution of the order parameter $S_{max}(\mathbf{k})/N$ with the density for $\alpha = 0.1$ (upper left), $\alpha = 0.2$ (upper right), $\alpha = 0.3$ (lower left) and $\alpha = 0.4$ (lower right).

the order of the crystal to stripe phase transition. In this case we have not detected a smooth decay of the second peak of the static structure factor by increasing the polarization angle of the dipoles. On the contrary, the second crystalline Bragg peak suddenly disappears when a slight change in the tilting angle near the transition point is made, thus indicating that the crystal to stripe phase transition is probably of first order.

At this point we have covered the whole range of densities and polarization angles that can be reliably spanned with our simulation methods. The full phase diagram of the 2D dipolar Bose system is shown in Fig. 4, where both the simulation points and the transition lines separating the different phases are depicted and separated from the collapse region where the system no longer exists. It is interesting to notice from the phase diagram that there are cuts at constant density in the range $nr_0^2 \in (290, 450)$ where by increasing the polarization angle from $\alpha = 0$ all the way to the collapse limit one can find the system in solid phase, then in a gaseous form, to finally jump into the stripe phase. All these changes are due to a delicate balance between the strength of the interaction and its anisotropy, which in some sense compete against each other when the polarization angle increases.

To summarize, using quantum Monte Carlo we have studied the phase diagram of bosonic tilted dipoles in 2D relying only on the Hamiltonian of the system. Our results show that at low densities the system is in the gas phase. When the density is increased and the tilting angle is below $\alpha \sim 0.45$ the system undergoes a first order phase transition and crystallizes. The anisotropy of the interaction influences the shape of the crystalline lattice by elongating the fundamental triangle in the direction where the dipole-dipole interaction is stronger. Beyond the critical point at $\alpha \sim 0.45$ a second order phase transition brings the system from the gas to a stripe phase.

The critical exponents of this second order transition are essentially independent of the polarization angle and are compatible with the 3D Ising universality class within the statistical uncertainty of our simulations. Remarkably, our results show that for large polarization angles the stripe phase can be observed experimentally at densities significantly lower than those required to reach the solid phase, and without any optical lattice [23]. Finally, at high densities and large tilting angles the system undergoes a first order phase transition from the crystal to the stripe phase. In this case, the slope of the transition line is extremely large and indicates that, due to the anisotropy of the interaction, the crystal phase of the system can become the most stable one only at extremely large densities that are nevertheless out of reach of our simulations.

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